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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The method of rank annihilation is shown to be a particular case of a more general method for quantitation in bilinear data arrays such as LC/UV, GC/MS or emission-excitation fluorescence. Generalized rank annihilation is introduced as a calibration method that allows for simultaneous quantitative determination of all of the analytes of interest in a mixture of unknowns. Only one calibration mixture is required. The bilinear spectra of both unknown and calibration sample must be obtained. Bilinear target factor analysis is introduced as a projection of a target bilinear matrix onto another principal component bilinear matrix space.		

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Generalized Rank Annihilation Factor Analysis

by

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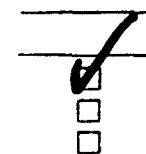
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Generalized Rank Annihilation Factor Analysis

Sir: The analytical chemist is frequently confronted with the problem of analyzing complex mixtures for which only concentrations of a few components are of interest. In these cases, it is desirable to be able to obtain quantitative information for the analytes of interest without concern for the rest of the components in the sample. Second order bilinear sensors, i.e. sensors that yield a two dimensional data matrix of the form $M_{ij} = \sum_k \beta_k x_{ik} y_{jk}$, are specially suited for this purpose, and the preferred technique for quantitation is known as rank annihilation factor analysis, RAFA (1,2). So far this method has been applied to excitation-emission fluorescence (1-3), LC/UV (4) and TLC-reflectance imaging spectrophotometry (5) with good results. It is important to realize that not all two dimensional techniques yield bilinear data arrays: e.g. 2D-NMR or MS/MS data in their raw forms are not bilinear.

A limitation of rank annihilation as originally formulated is that an iterative solution requiring many matrix diagonalizations is necessary (1). Lorber (6) has reported a non-iterative solution presenting the problem as a generalized eigenvalue-eigenvector equation for which a direct solution is found by using the singular value decomposition. With his method, to obtain the concentrations of the p analytes of interest in the sample, its bilinear spectrum and the p calibration spectra for each pure analyte must be recorded to obtain the concentrations. Analysis for each analyte requires a separate calculation. This letter presents the generalized rank annihilation method, of which Lorber's non-iterative method is only a particular case, that allows simultaneous quantitation of analytes in a sample using just



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one bilinear calibration spectrum obtained from a mixture of standards, one standard for each analyte.

Generalized rank annihilation can determine the bilinear spectrum and the relative concentration for each analyte in the unknown mixture. The calculated spectra are next matched to those of the standards. It is then straightforward to determine the actual concentration of each analyte from its relative concentration and the concentration of the corresponding standard. The full bilinear spectrum of each analyte is not actually required for identification. One need only use a single order (e.g. only the UV spectrum in the LC/UV case) for the match. This is an unusual type of analysis as in most cases, analyte concentrations are estimated one at a time thereby precluding identification.

THEORY AND DISCUSSION

Any bilinear data matrix M can be expressed as a linear combination of the n pure-component, bilinear spectra \mathcal{M}_k :

$$M = \sum_k^n \beta_k \mathcal{M}_k \quad \text{where } \mathcal{M}_k = x_k y_k^T ; (\mathcal{M}_{ij})_k = x_{ik} y_{jk} \quad (1)$$

The x_k are column vectors with information in one order, e.g. excitation spectra, and the y_k^T are row vectors with information in the second order, e.g. emission spectra. If we define the \mathcal{M}_k as unitary-concentration, pure-component, bilinear spectra, β_k is the concentration of the k^{th} compound in M . We can rewrite eq 1 in matrix notation as

$$M = X B Y^T \quad (2)$$

where \mathbf{X} is a matrix whose columns are the $n \times_k$ vectors, \mathbf{Y}^T is a matrix whose rows are the $n \times_k^T$ vectors and \mathbf{B} is a diagonal matrix with diagonal elements that are the concentrations, β_k .

In general we will have two data matrices, the unknown concentrations data matrix \mathbf{M} and the calibration data matrix \mathbf{N} . The bilinear calibration data matrix \mathbf{N} can similarly be represented in matrix notation as

$$\mathbf{N} = \mathbf{X} \xi \mathbf{Y}^T \quad (3)$$

where \mathbf{X} and \mathbf{Y}^T are the same matrices defined for eq 2 and ξ is a diagonal matrix whose diagonal elements are the concentrations ξ_k for the calibration matrix.

The matrices \mathbf{M} and \mathbf{N} have in common the \mathbf{X} and \mathbf{Y}^T blocks, e.g. the excitation and emission spectra are the same, differing only in their concentration matrices, \mathbf{B} and ξ respectively. Therefore, solving for \mathbf{X} in eq 2 and eq 3 we obtain

$$\mathbf{X} \mathbf{B} = \mathbf{M} (\mathbf{Y}^T)^+ \quad (4)$$

$$\mathbf{X} \xi = \mathbf{N} (\mathbf{Y}^T)^+ \quad (5)$$

where $(\mathbf{Y}^T)^+$ represents the pseudoinverse (7) of the matrix \mathbf{Y}^T . Now we right-multiply eq 4 by ξ and eq 5 by \mathbf{B} and combine to get:

$$\mathbf{N} (\mathbf{Y}^T)^+ \mathbf{B} = \mathbf{M} (\mathbf{Y}^T)^+ \xi \quad (6)$$

defining $\mathbf{Z} \equiv (\mathbf{Y}^T)^+$,

$$\mathbf{N} \mathbf{Z} \mathbf{B} = \mathbf{M} \mathbf{Z} \xi \quad (7)$$

We only know \mathbf{M} , \mathbf{N} and ξ , thus we must to solve for \mathbf{Z} and \mathbf{B} . Eq (7) is similar to the generalized eigenvalue-eigenvector problem, but can not be solved by standard methods since \mathbf{N} and \mathbf{M} are not necessarily square matrices. A solution of this equation will be discussed in the next sections, for the following different possible cases:

[1] The calibration data matrix **N** has just *one* component, that is present in the sample data matrix **M**,

$$\text{diagonal}(\beta) = \{\beta_1, \beta_2, \dots, \beta_n\} \quad n \geq 1 \quad (8)$$

$$\text{diagonal}(\xi) = \{\xi_1, 0, \dots, 0\} \quad (9)$$

This is the standard RAFA problem as discussed by Lorber (6).

[2] The calibration data matrix **N** has *several* components, that are a *subset* of the components present in the sample data matrix **M**,

$$\text{diagonal}(\beta) = \{\beta_1, \beta_2, \dots, \beta_r, \beta_{r+1}, \beta_{r+2}, \dots, \beta_{r+s}\} \quad r \geq 0 \quad (10)$$

$$\text{diagonal}(\xi) = \{0, 0, \dots, 0, \xi_{r+1}, \xi_{r+2}, \dots, \xi_{r+s}\} \quad s \geq 1 \quad (11)$$

Here, *r* is the number of components in the sample **M** that are not present in the calibration **N**, and *s* is the number of common components.

[3] The components in the sample data matrix **M** are a subset of the components present in the calibration data matrix **N**,

$$\text{diagonal}(\beta) = \{\beta_1, \beta_2, \dots, \beta_s, 0, \dots, 0\} \quad s \geq 1 \quad (12)$$

$$\text{diagonal}(\xi) = \{\xi_1, \xi_2, \dots, \xi_s, \xi_{s+1}, \dots, \xi_{s+t}\} \quad t \geq 1 \quad (13)$$

Again, *s* is the number of common components, and *t* is the number of components in the calibration **N** that are absent from the sample **M**.

[4] The most general case would be when there are analytes in the unknown sample that are not present in the calibration sample and vice versa,

$$\text{diagonal}(\beta) = \{\beta_1, \beta_2, \dots, \beta_r, \beta_{r+1}, \beta_{r+2}, \dots, \beta_{r+s}, 0, \dots, 0\} \quad (14)$$

$$\text{diagonal}(\xi) = \{0, 0, \dots, 0, \xi_{r+1}, \xi_{r+2}, \dots, \xi_{r+s}, \xi_{r+s+1}, \dots, \xi_{r+s+t}\} \quad (15)$$

Here, *r* is the number of components in the sample **M** that are not present in the calibration **N**, *s* is the number of common components, and *t* is the number of components in the calibration data matrix **N** that are absent in the unknown sample **M**.

[1] FIRST CASE: One Component Quantitation

In this case, the calibration data matrix N has just one component, \mathbf{A}_k , that is also present in the sample data matrix. The solution for this case has been reported by Lorber (6) and will be included here for completeness.

The first step in solving eq 7 is to apply principal components analysis (8) to the sample matrix M , and then express the matrices in terms of these principal components. The principal components of M are obtained by applying singular value decomposition (7)

$$M = U S V^T \quad (16)$$

where

$$M V = S U \quad (17)$$

$$M^T U = S V \quad (18)$$

$$M^T M V = S^2 V \quad \text{eigen-equations in } V \text{ space.} \quad (19)$$

$$M M^T U = S^2 U \quad \text{eigen-equations in } U \text{ space.} \quad (20)$$

The next step is to estimate the number of principal components that are significant using abstract factor analysis (8) or cross validation (9,10). In the ideal case, this number is equal to the number of components n in the sample mixture. The number of significant principal components will allow reduction to the deterministic information contained in the M matrix, with random error discarded in the lesser factors. To do this, a new matrix \underline{M} is generated from the first n "significant" columns of U , V and the upper left corner n by n part of S ,

$$\underline{M} = \underline{U} \underline{S} \underline{V}^T \quad (21)$$

Now eq 7 can be rewritten as

$$N Z B = \underline{M} Z \xi = \underline{U} \underline{S} \underline{V}^T Z \xi \quad (22)$$

If we substitute $Z = \underline{Y} \underline{S}^{-1} Z^*$, where $Z^* = \underline{S} \underline{Y}^T Z$

$$\underline{N} (\underline{Y} \underline{S}^{-1} Z^*) \underline{B} = \underline{U} \underline{S} \underline{Y}^T (\underline{Y} \underline{S}^{-1} Z^*) \xi \quad (23)$$

using the orthogonality properties of \underline{Y} , $\underline{Y}^T \underline{Y} = \underline{I}$ = Identity matrix in the upper left n by n corner and zeros in the rest, so:

$$\underline{N} \underline{Y} \underline{S}^{-1} Z^* \underline{B} = \underline{U} \underline{S} \underline{I} \underline{S}^{-1} Z^* \xi = \underline{U} (\underline{S} \underline{S}^{-1}) Z^* \xi \quad (24a)$$

which reduces to

$$(\underline{N} \underline{Y} \underline{S}^{-1}) Z^* \underline{B} = \underline{U} Z^* \xi \quad (24b)$$

Left-multiplying by \underline{U}^T and right-multiplying by \underline{B}^{-1} gives

$$(\underline{U}^T \underline{N} \underline{Y} \underline{S}^{-1}) Z^* \underline{B} \underline{B}^{-1} = (\underline{U}^T \underline{U}) Z^* \xi \underline{B}^{-1} = Z^* \lambda \quad \lambda \equiv \xi \underline{B}^{-1} \quad (25a)$$

or, finally,

$$(\underline{U}^T \underline{N} \underline{Y} \underline{S}^{-1}) Z^* = Z^* \lambda \quad (25b)$$

which is the usual eigenvalue-eigenvector equation, because the matrix $(\underline{U}^T \underline{N}_k \underline{Y} \underline{S}^{-1})$ is square. The eigenvectors Z^* are not perpendicular because the matrix $(\underline{U}^T \underline{N}_k \underline{Y} \underline{S}^{-1})$ is not symmetric. Because the rank of \underline{N} is one, there will be $p-1$ zero solutions for the eigenvalues λ_k . Therefore, the only non-zero solution will be equal to the trace of the matrix $(\underline{U}^T \underline{N}_k \underline{Y} \underline{S}^{-1})$. By calculating the trace of this matrix, i.e. λ_k , the concentration β_k of the k^{th} component is solved directly as $\beta_k = \xi_k / \lambda_k$.

If the unknown sample does not have the component that is present in the calibration sample, we cannot expand \underline{N} in terms of \underline{X} and \underline{Y} (eq 3), therefore eq 25b is not valid. This is an example of the fourth case introduced in the previous section, which will be considered later in this paper. In practice, a non-zero concentration value β_k will be obtained, so the validity of eq 3 must be verified before applying eq 25b. Using target factor analysis (8,11), modified for bilinear data, it is possible to check if \underline{N} is included in \underline{M} (see appendix for the details of bilinear target factor analysis). The projection matrices $\underline{U} \underline{U}^T$ and $\underline{Y} \underline{Y}^T$ should leave \underline{N} unchanged:

$$\underline{U} \underline{U}^T \underline{N} \underline{V} \underline{V}^T = \underline{N} \quad (26)$$

As pointed out by Lorber (6), if the calibration matrix \underline{N} has more than one component, i.e. its rank is greater than one, several solutions will be obtained for the concentrations $\beta_1, \beta_2, \dots, \beta_n$, but there will be no way to match which concentration corresponds to which chemical component. The proposed alternative is to obtain the spectrum of all the components separately, and estimate their concentration one by one. A solution to this problem is described in the next section, using the eigenvectors matrix \underline{Z} in eq 7, which was defined as the pseudoinverse of the \underline{Y}^T , i.e. the generalized inverse of the pure component's emission spectra.

[2] SECOND CASE: Simultaneous Quantitation of Several Components

In this case, the calibration data matrix \underline{N} has several components, that are a subset of the components present in the sample data matrix \underline{M} . In the first place, it is necessary to check that the components in \underline{N} are a subset of the components present in the sample data matrix \underline{M} , applying bilinear target factor analysis to the matrix \underline{N} , i.e. eq 26 should be true.

If more than one component is represented in the calibration matrix, eq 25b has several non-zero eigenvalues. The solution is a set of eigenvalues λ and their corresponding eigenvectors \underline{Z}^* . The eigenvectors allow us to calculate the pure spectra matrices \underline{X} and \underline{Y}^T , e.g. excitation and emission spectra:

$$\underline{Z}^* = \underline{S} \underline{V}^T \underline{Z} = \underline{S} \underline{V}^T (\underline{Y}^T)^+ \quad (27)$$

$$\underline{Y}^T = (\underline{V} \underline{S}^{-1} \underline{Z}^*)^+ \quad (28)$$

Using the definition of $\underline{M} = \underline{X} \underline{B} \underline{Y}^T = \underline{U} \underline{S} \underline{V}^T$

$$XB = M(Y^T)^+ = U S Y^T Y S^{-1} Z^* = U Z^* \quad (29)$$

The eigenvalues λ_k are the ratio of concentrations ξ_k/β_k for each component, i.e. calibration/unknown. Having the pure spectra x_k or y_k^T , it is easy to match which concentration ξ_k corresponds to which ratio λ_k , therefore the concentrations β_k can be estimated $\beta_k = \xi_k/\lambda_k$.

[3] THIRD CASE: Calibration as a Base

When the sample data matrix M is a subset of the components in the calibration N , we must invert the procedure. The principal components of the matrix M do not form a basis for the representation of the matrix N , therefore eq 25b is not valid in this case. The principal components of N are estimated $N = U_N S_N Y_N^T$, and equations similar to eq 25b, 28, 29 are obtained:

$$(U_N^T M Y_N S_N^{-1}) Z_N^* = Z_N^* \lambda_N \quad (30)$$

$$Y^T = (Y_N S_N^{-1} Z_N^*)^+ \quad (31)$$

$$XB = U_N Z_N^* \quad (32)$$

The eigenvalues $(\lambda_N)_k$ are not defined as they were before. Now the $(\lambda_N)_k$ are the ratio of concentrations β_k/ξ_k for each component, i.e. unknown sample/calibration.

Bilinear target factor analysis can be used to test instances of the third case. The projection of the matrix M in the spaces defined by N should leave M unchanged:

$$U_N U_N^T M Y_N Y_N^T = M \quad (33)$$

If both this test and eq 26 fail, then we are dealing with the fourth case, discussed in the next section. In practice, the third case can be solved using

principal components analysis or multiple linear regression, because the spectra of all the components are known.

[4] FOURTH CASE: The General Condition

In this case, the calibration sample will have some components that are not present in the unknown sample, and there will be some components in this unknown sample not present in the calibration sample. Projection of one matrix onto the principal components of the other matrix will change its information; eq 25b and eq 30 will not be valid.

A solution to this problem can be obtained using the principal components of the sum of the matrices M and N , defining $W \equiv M + N$,

$$W = \underline{U}_W \underline{S}_W \underline{Y}_W^T \quad (34)$$

$$(\underline{U}_W^T M \underline{Y}_W \underline{S}_W^{-1}) Z_W^* = Z_W^* \lambda_W \quad (35)$$

$$Y^T = (\underline{Y}_W \underline{S}_W^{-1} Z_W^*)^+ \quad (36)$$

$$XB = \underline{U}_W Z_W^* \quad (37)$$

The eigenvalues λ_k are the ratio of concentrations $\beta_k/(\xi_k + \beta_k)$. For all the components present in both mixtures, the concentration in the unknown is $\beta_k = \lambda_k \xi_k / (1 - \lambda_k)$. When one component is not present in the calibration sample, $\xi_k = 0$, and $\lambda_k = 1$.

The solution presented for this case can be applied to all the previous cases, and no testing with target factor analysis is necessary. An artificial matrix W is generated to perform the calculations. This suggests that one could instead generate the W matrix simply by making a single standard addition containing known amounts of all analytes to the unknown sample. In this way the calibration mixture is added to the unknown mixture, and the W matrix is measured directly. Quantitation by RAFA with

the standard addition method (SAM) has been discussed by Lorber (14) for single analyte addition. This procedure would extend the applicability of his method to the quantitation of several analytes at a time, correcting for matrix effects and thereby represents an extension of the generalized standard addition method, GSAM (12,13), to second-order tensor data.

If we have several calibration matrices N_1, N_2, \dots, N_q , we can apply the method to all of them, one at a time, or we can handle it as a three way factor analysis problem, using all of the information in one calculation. We are currently working in this problem, which will be the subject of another publication.

APPENDIX

Target Factor Analysis (8,11) can be applied to bilinear data in a similar way that it is used to one dimensional data. For the test vectors x_i or y_i , TFA can be expressed as:

$$\underline{U} \underline{U}^T x_i = x_i \quad \text{or} \quad y_i^T \underline{V} \underline{V}^T = y_i^T \quad (38)$$

every test vector x_i or y_i generates a predicted target vector \hat{x}_i or \hat{y}_i . If the test vectors are present in the matrix M , i.e. if the i^{th} -component, which spectrum is $x_i y_i$, is present in M , then the predicted target vectors should be equal to the test vectors: $\hat{x}_i = x_i$; $\hat{y}_i = y_i$; therefore

$$\underline{U} \underline{U}^T x_i = x_i \quad \text{or} \quad y_i^T \underline{V} \underline{V}^T = y_i^T \quad (39)$$

using the definition of X and Y we can similarly write

$$\underline{U} \underline{U}^T X = X \quad Y^T \underline{V} \underline{V}^T = Y^T \quad (40)$$

now, if $N = X \otimes Y^T$, then

$$\underline{U} \underline{U}^T N \underline{V} \underline{V}^T = (\underline{U} \underline{U}^T X) \otimes (Y^T \underline{V} \underline{V}^T) = X \otimes Y^T = N \quad (41)$$

this is,

$$\underline{U} \underline{U}^T N \underline{V} \underline{V}^T = N. \quad (42)$$

this equation defines bilinear target factor analysis. Note that

$$\underline{U} \underline{U}^T N = N. \quad \text{and} \quad N \underline{V} \underline{V}^T = N. \quad (43)$$

in practice, due to random noise, equations 42-44 are approximate.

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